

=> d que

L2 505403 SEA FILE=REGISTRY ABB=ON PLU=ON NCNC3/ES
 L3 392874 SEA FILE=REGISTRY ABB=ON PLU=ON NC2NC2/ES
 L4 882977 SEA FILE=REGISTRY ABB=ON PLU=ON L2 OR L3
 L6 713083 SEA FILE=REGISTRY ABB=ON PLU=ON L4 AND ((O/ELS AND S/ELS) OR
 O>1)
 L12 522345 SEA FILE=REGISTRY ABB=ON PLU=ON (L6 AND NC=1) NOT (P/ELS OR
 SI/ELS)
 L14 472811 SEA FILE=REGISTRY ABB=ON PLU=ON L12 AND NRS<5
 L16 197390 SEA FILE=REGISTRY ABB=ON PLU=ON L14 AND NC2NC2/ES
 L19 275421 SEA FILE=REGISTRY ABB=ON PLU=ON L14 NOT L16
 L41 STR

19 21
 G4 G4
 2
 G1=Hy G2 CH2G3 CH2·CH2G3 CH2·CH2·CH2G3 O @18
 1 3 @4 5 @6 7 8 @9 10 11 12
 G4
 20
 CH2·CH2·CH2·CH2G3
 @13 14 15 16 17

VAR G1=O/S
 VAR G2=4/6/9/13
 VAR G3=X/18
 VAR G4=H/X/OH/NO2/AK/O/CY/N/S
 NODE ATTRIBUTES:
 CONNECT IS E1 RC AT 18
 DEFAULT MLEVEL IS ATOM
 GGCAT IS MCY UNS AT 2
 DEFAULT ECLEVEL IS LIMITED
 ECOUNT IS E4 C E2 N AT 2

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 21

STEREO ATTRIBUTES: NONE

L43 279 SEA FILE=REGISTRY SUB=L16 SSS FUL L41
 L45 1824 SEA FILE=REGISTRY SUB=L19 SSS FUL L41
 L46 2103 SEA FILE=REGISTRY ABB=ON PLU=ON L43 OR L45
 L47 2110 SEA FILE=HCAPLUS ABB=ON PLU=ON L46
 L48 1615 SEA FILE=HCAPLUS ABB=ON PLU=ON L47 NOT PY>1996

=> d ibib abs hitstr 1-20

L48 ANSWER 1 OF 1615 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1997:356424 HCAPLUS
 DOCUMENT NUMBER: 126:334395
 TITLE: Pyrimidinone derivative for treatment of senescence,
 diabetic- and radiation-induced slow-healing wound
 INVENTOR(S): Izmajlov, Gennadij Alekseevich; Izmajlov, Sergej
 Gennadievich; Reznik, Vladimir Savvich; Gorbunov,
 Sergej Mikhajlovich; Zuev, Yuriy Alekseevich;

Only first
 20 References
 Printed. I
 can print more
 if you need
 them.

PATENT ASSIGNEE(S): Gilmutdinov, Il Garafeevich
 SOURCE: Institut Organicheskoy I Fizicheskoy Khimii, Estonia
 Russ., 163 pp. From: Izobreteniya 1996, (20), 163.
 CODEN: RUXXE7
 DOCUMENT TYPE: Patent
 LANGUAGE: Russian
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
AB	RU 2063752	C1	19960720	RU 1993-29221	19930608
IT	Title only translated.				
	14716-32-6				
	RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)				
	(pyrimidinone deriv. for treatment of senescence and slow-healing wounds)				
RN	14716-32-6	HCAPLUS			
CN	2(1H)-Pyrimidinone, 1-(2-hydroxyethyl)-4,6-dimethyl- (8CI, 9CI) (CA INDEX NAME)				

Claim 26:

X = $\text{C}=\text{O}$

Y = $\text{C}=\text{C}$

Z = $\text{C}=\text{C}$

R1 = Alkyl (Me)

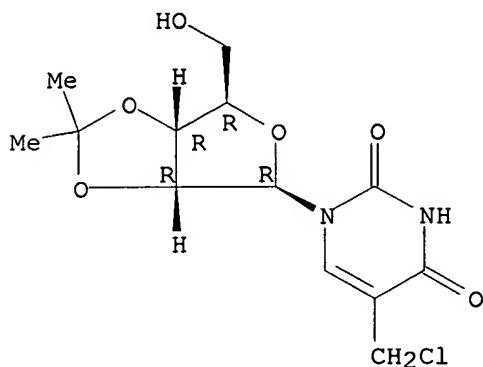
R2 = Alkyl (Me)

R3 = H

L48 ANSWER 2 OF 1615 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1997:211709 HCAPLUS
 DOCUMENT NUMBER: 126:251346
 TITLE: Synthesis of some aminonaphthalene and 5-substituted uracil nucleosides derivatives
 AUTHOR(S): Sayed Ahmed, A. F.; Milad, A.
 CORPORATE SOURCE: Faculty of Science, Zagazig University, Zagazig, Egypt
 SOURCE: Egyptian Journal of Pharmaceutical Sciences (1996), 37(1-6), 493-500
 CODEN: EJPSBZ; ISSN: 0301-5068
 PUBLISHER: National Information and Documentation Centre
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Some aminonaphthalene nucleosides were prep'd. by the reaction of both of 1-amino, 1-aminomethyl, 1,5-diamino and 2,6-bis(aminomethyl)naphthalene derivs. with 2,3,5-tri-O-acetylribofuranosyl chloride. On the other hand, the reactions of 2',3'-O-isopropylidene-5-aminouridine and its 5-aminomethyl analog with gluconolactone and the reactions of 2',3'-O-isopropylidene-5-chloromethyluridine with sodium N-methyltaurinate have been described.
 IT **89148-09-4**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of aminonaphthalene uracil nucleosides via coupling reaction)
 RN 89148-09-4 HCAPLUS

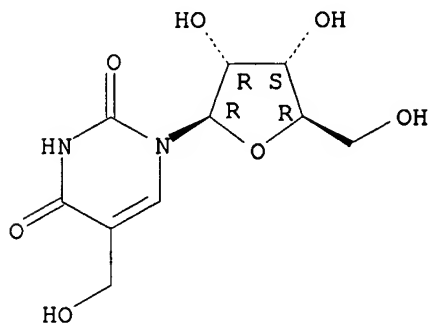
CN Uridine, 5-(chloromethyl)-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L48 ANSWER 3 OF 1615 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1997:211491 HCAPLUS
 DOCUMENT NUMBER: 126:264305
 TITLE: Synthesis of some uridine and cytidine derivatives
 AUTHOR(S): Sayed Ahmed, A. F.
 CORPORATE SOURCE: Chem. Dep., Zagazig Univ., Zagazig, Egypt
 SOURCE: Egyptian Journal of Pharmaceutical Sciences (1996),
 37(1-6), 303-311
 CODEN: EJPSBZ; ISSN: 0301-5068
 PUBLISHER: National Information and Documentation Centre
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Some modified nucleosides were prepd. from 5, 6-disubstituted uridine,
 5-substituted cytidine and cytidine. Different nucleophilic substitution
 reactions were carried out in alk. or neutral medium. Some of these
 reactions describe ring formation.
 IT **30414-00-7**, 5-Hydroxymethyluridine **188842-72-0**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of uridines and cytidines using nucleophilic substitution)
 RN 30414-00-7 HCAPLUS
 CN Uridine, 5-(hydroxymethyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

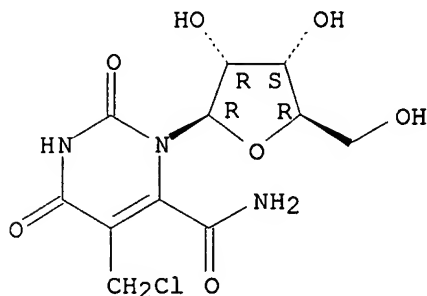
Absolute stereochemistry.



RN 188842-72-0 HCAPLUS

CN Uridine, 6-(aminocarbonyl)-5-(chloromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



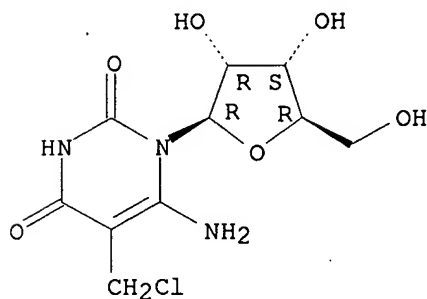
IT 188842-61-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of uridines and cytidines using nucleophilic substitution)

RN 188842-61-7 HCAPLUS

CN Uridine, 6-amino-5-(chloromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L48 ANSWER 4 OF 1615 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1997:146915 HCAPLUS

DOCUMENT NUMBER: 126:255385

TITLE: Synthesis and controlled-release of polymer drug using lactic acid-phosphate copolymer as drug carriers

AUTHOR(S): Fang, Chang-Lie; Li, Bing; Liu, Zhen-Hua; Zhuo, Ren-Xi
CORPORATE SOURCE: Dep. Chem., Wuhan Univ., Wuhan, 430072, Peop. Rep. China

SOURCE: Gaodeng Xuexiao Huaxue Xuebao (1996), 17(11), 1788-1791

CODEN: KTHPDM; ISSN: 0251-0790

PUBLISHER: Gaodeng Jiaoyu Chubanshe

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB Controlled-release polymer drugs, using 5-FU as model drug, lactic acid-phosphate copolymers as polymer drug carriers, were prepd. The copolymers were characterized by 1H NMR, IR and UV spectroscopy. The contents of 5-FU were detd. by UV spectroscopy. The drug showed controlled-release in vitro and the copolymer compn. [i.e. variations in

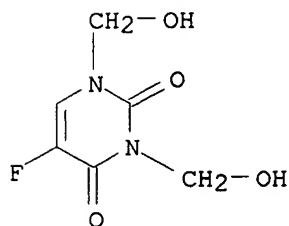
DL-lactic acid: TMP ratios] had profound effect on the drug release rate.

IT 74179-14-9

RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis and controlled-release of polymer drug using lactic acid-phosphate copolymer as drug carriers)

RN 74179-14-9 HCAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 5-fluoro-1,3-bis(hydroxymethyl)- (9CI) (CA INDEX NAME)

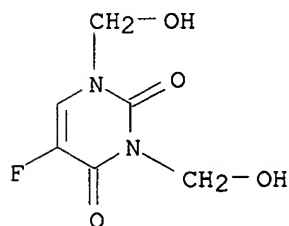


IT 74179-14-9DP, reaction product with chlorinated trimethylene phosphonate and lactide

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and controlled-release of polymer drug using lactic acid-phosphate copolymer as drug carriers)

RN 74179-14-9 HCAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 5-fluoro-1,3-bis(hydroxymethyl)- (9CI) (CA INDEX NAME)



L48 ANSWER 5 OF 1615 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1997:106719 HCAPLUS

DOCUMENT NUMBER: 126:144265

TITLE: A novel type of rigid macrocycle with bis(3-uracilyl)methane and hexadiyne units The uracilophane

AUTHOR(S): Caplar, Vesna; Tumir, Lidija; Zinic, Mladen
CORPORATE SOURCE: Laboratory of Supramolecular and Nucleoside Chemistry, Department of Chemistry, Ruder Boskovic Institute, Zagreb, 10001, Croatia

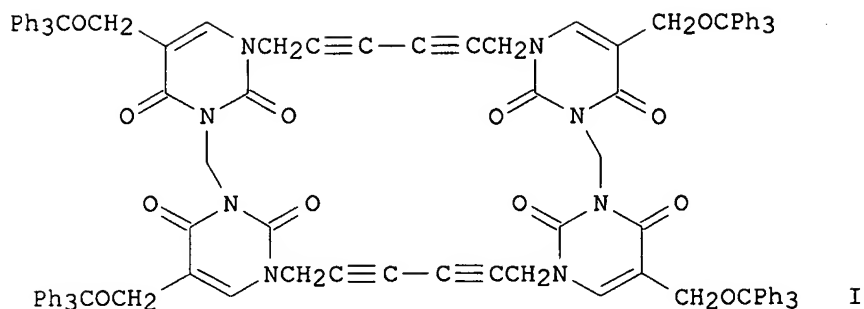
SOURCE: Croatica Chemica Acta (1996), 69(4), 1617-1631
CODEN: CCACAA; ISSN: 0011-1643

PUBLISHER: Croatian Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



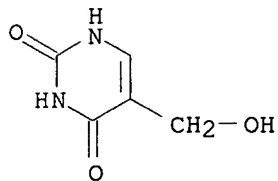
AB Synthesis of the uracilophane I, constructed from two bis(3-uracilyl)methane units and two hexadiyne bridges connecting uracil N(1)-atoms, is described. The conformational properties of I investigated by mol. dynamics revealed low energy conformations with partly or fully stacked phenyl-uracil or phenyl-Ph pairs.

IT **4433-40-3**, 5-Hydroxymethyluracil

RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. and conformation of uracilophane)

RN 4433-40-3 HCAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 5-(hydroxymethyl)- (9CI) (CA INDEX NAME)

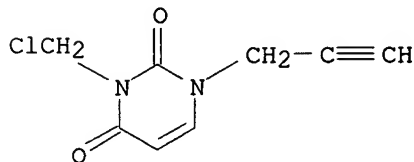


IT **168413-07-8P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and conformation of uracilophane)

RN 168413-07-8 HCAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 3-(chloromethyl)-1-(2-propynyl)- (9CI) (CA INDEX NAME)

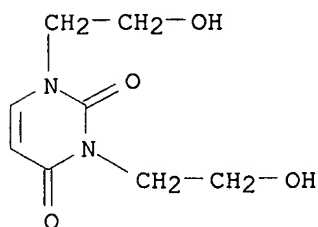


L48 ANSWER 6 OF 1615 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1997:38586 HCAPLUS
 DOCUMENT NUMBER: 126:54871
 TITLE: 1,3-Bis(2-hydroxyethyl)uracil showing inotropic activity
 INVENTOR(S): Grinevich, Aleksandr Iosifovich; Vojtsekhovskaya, Oksana Mikhajlovna; Chekman, Ivan Sergeevich; Puzenkina, Ninel Nikolaevna; Podgornyj, Andrej Vadimovich; Gorchakova, Nadezhda Aleksandrovna; Nizhenkovskaya, Irina Vladimirovna
 PATENT ASSIGNEE(S): Kievskij Meditsinskij Institut Im.Akad.A.A.Bogomoltsa, Ukraine
 SOURCE: Russ. From: Izobreteniya 1996, (7), 168.
 CODEN: RUXXE7
 DOCUMENT TYPE: Patent
 LANGUAGE: Russian
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

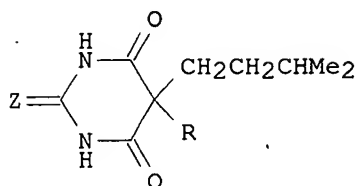
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
RU 2055581	C1	19960310	RU 1992-5051178	19920706
PRIORITY APPLN. INFO.:			SU 1992-5051178	19920706

AB Title only translated.
 IT 711-66-0, 1,3-Bis(2-hydroxyethyl)uracil
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (1,3-bis(2-hydroxyethyl)uracil as inotropic agent)
 RN 711-66-0 HCAPLUS
 CN 2,4(1H,3H)-Pyrimidinedione, 1,3-bis(2-hydroxyethyl)- (9CI) (CA INDEX NAME)



L48 ANSWER 7 OF 1615 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1996:735413 HCAPLUS
 DOCUMENT NUMBER: 126:42200
 TITLE: Comparison between the metabolism of branched-chain barbiturates and that of their sulfur-containing analogs
 AUTHOR(S): Yebga, A.; Menager, S.; Verite, P.; Combet Farnoux, C.; Lafont, O.
 CORPORATE SOURCE: Laboratoire de Pharmacochimie Biopharmacie, Faculte de Medecine et de Pharmacie, Saint Etienne du Rouvray Cedex, 76803, Fr.
 SOURCE: Acta Technologiae et Legis Medicamenti (1995), 6(3, Suppl., XXI Congresso Internazionale della Societa

PUBLISHER: Farmaceutica del Mediterraneo Latino, 1994), 536-539
 DOCUMENT TYPE: CODEN: ATLMEQ; ISSN: 1121-2098
 LANGUAGE: Maccari
 Journal
 French
 GI



I

AB Four barbiturates or thiobarbiturates (I; Z = O or S; R = Et or Pr) were given orally to rats at 20 mg/kg/day for 8-10 days, and the urines were analyzed for metabolites by ¹H-NMR spectrometry, mass spectrometry, and gas chromatog. The greater lipophilicity of the thiobarbiturates than of the barbiturates did not cause an increase in the amt. of drug metabolized. The .beta.-oxidn. of the Et chain of amobarbital (I; Z = O; R = Et), which is the 1st step in the opening of the pyrimidinetrione ring by intramol. alcoholysis, did not take place in the case of the S-contg. analog. Desulfuration was not the principal metabolic pathway of the thiobarbiturates. With the barbiturates, there was no carboxylated metabolite formed by the .omega.-oxidn. of the side chains, contrary to what has been described for the thiobarbiturates.

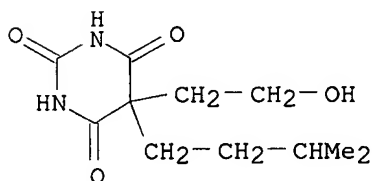
IT 68160-58-7

RL: BPR (Biological process); BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative); PROC (Process)

(metab. of barbiturates and thiobarbiturates resulting in formation of)

RN 68160-58-7 HCAPLUS

CN 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(2-hydroxyethyl)-5-(3-methylbutyl)-
 (9CI) (CA INDEX NAME)



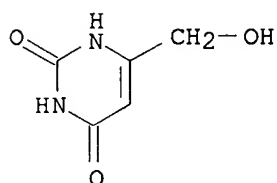
L48 ANSWER 8 OF 1615 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:733960 HCAPLUS

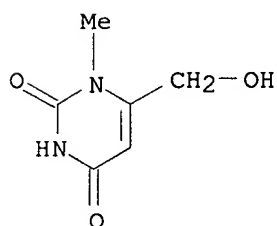
DOCUMENT NUMBER: 126:103814

TITLE: Hydrogen-bonded complexes of diaminopyridines and diaminotriazines: opposite effect of acylation on complex stabilities. [Erratum to document cited in CA125:194913]

AUTHOR(S): Beijer, Felix H.; Sijbesma, Rint P.; Vekemans, Jef. A. J. M.; Meijer, E. W.; Kooijman, Huub; Spek, Anthony L.
 CORPORATE SOURCE: Department of Organic Chemistry, Eindhoven University of Technology, Eindhoven, 5600 MB, Neth.
 SOURCE: Journal of Organic Chemistry (1996), 61(26), 9636
 CODEN: JOCEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The authors make corrections to pages 6374-6378.
 IT **22126-44-9**
 RL: PEP (Physical, engineering or chemical process); PROC (Process) (opposite effect of acylation on stabilities of hydrogen-bonded complexes of diaminopyridines and diaminotriazines (Erratum))
 RN 22126-44-9 HCAPLUS
 CN 2,4(1H,3H)-Pyrimidinedione, 6-(hydroxymethyl)- (9CI) (CA INDEX NAME)

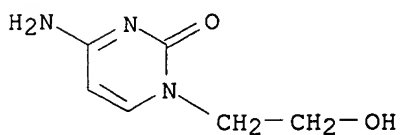


IT **2476-13-3P**
 RL: PEP (Physical, engineering or chemical process); PNU (Preparation, unclassified); PRP (Properties); PREP (Preparation); PROC (Process) (opposite effect of acylation on stabilities of hydrogen-bonded complexes of diaminopyridines and diaminotriazines (Erratum))
 RN 2476-13-3 HCAPLUS
 CN 2,4(1H,3H)-Pyrimidinedione, 6-(hydroxymethyl)-1-methyl- (9CI) (CA INDEX NAME)

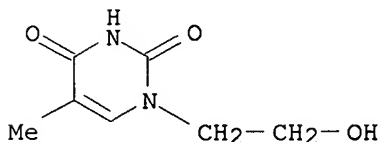


L48 ANSWER 9 OF 1615 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1996:733958 HCAPLUS
 DOCUMENT NUMBER: 126:131724
 TITLE: Synthesis of L-Dioxolane Nucleosides and Related Chemistry. [Erratum to document cited in CA122:188012]
 AUTHOR(S): Liang, Chengyi; Lee, Doo Won; Newton, M. Gary; Chu, Chung K.
 CORPORATE SOURCE: Department of Medicinal Chemistry, College of Pharmacy, Athens, GA, 30602, USA

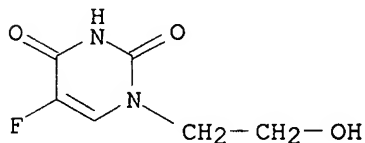
SOURCE: Journal of Organic Chemistry (1996), 61(26), 9634
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Scheme 2 is cor. The corresponding index entries have been cor.
accordingly.
IT 22441-50-5P 22441-51-6P 53540-73-1P
55343-20-9P 161469-40-5P 161469-41-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and rearrangement and ring cleavage of dioxolane nucleosides
(Erratum))
RN 22441-50-5 HCAPLUS
CN 2(1H)-Pyrimidinone, 4-amino-1-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)



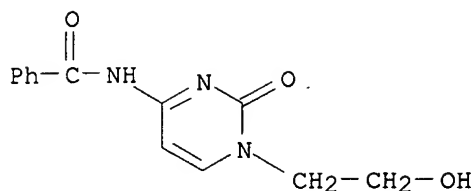
RN 22441-51-6 HCAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 1-(2-hydroxyethyl)-5-methyl- (9CI) (CA INDEX NAME)



RN 53540-73-1 HCAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 5-fluoro-1-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)

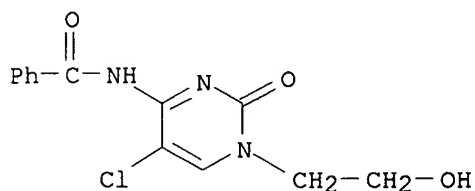


RN 55343-20-9 HCAPLUS
CN Benzamide, N-[1,2-dihydro-1-(2-hydroxyethyl)-2-oxo-4-pyrimidinyl]- (9CI)
(CA INDEX NAME)



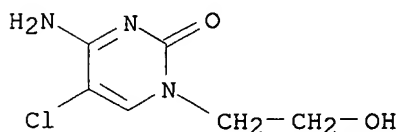
RN 161469-40-5 HCAPLUS

CN Benzamide, N-[5-chloro-1,2-dihydro-1-(2-hydroxyethyl)-2-oxo-4-pyrimidinyl]-
(9CI) (CA INDEX NAME)



RN 161469-41-6 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-5-chloro-1-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)



L48 ANSWER 10 OF 1615 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:730649 HCAPLUS

DOCUMENT NUMBER: 126:74661

TITLE: Metallocene-nucleobase conjugates. Synthesis, structure and nucleic acid binding

AUTHOR(S): Price, Clayton; Aslanoglu, Mehmet; Isaac, Christian J.; Elsegood, Mark R. J.; Clegg, William; Horrocks, Benjamin R.; Houlton, Andrew

CORPORATE SOURCE: Department Chemistry, University Newcastle upon Tyne, Newcastle upon Tyne, NE1 7RU, UK

SOURCE: Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1996), (21), 4115-4120
CODEN: JCDTBI; ISSN: 0300-9246

PUBLISHER: Royal Society of Chemistry

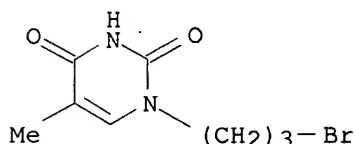
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The ferrocenylnucleobase conjugates [cyclic] [Fe(.eta.5-C5H5){.eta.5-C5H4CH2NMe2CH2CH2CH2NC(O)NHC(O)CMeCH}][BF4] 1 and [Fe(.eta.5-C5H5){.eta.5-C5H4CH2[C5H2N4(NH2)]}] 2 of thymine and adenine resp., have been prepd. and their crystal and mol. structures detd. The mol. packing of the two compds. differs markedly in terms of intermol. hydrogen-bonding

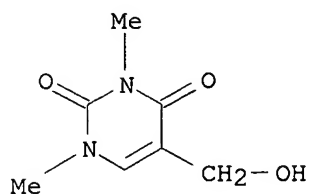
interactions. In 1 such interactions are confined to discrete cation.cntdot..cntdot..cntdot.anion.cntdot..cntdot..cntdot.solvate units, whereas in 2 the hydrogen-bonding patterns are extensive and involve both the Watson-Crick and Hoogsteen donor and acceptor sites. Electrochem. studies of the interaction of 1 with nucleic acids showed that the incorporation of this single nucleoside base with the metallocene moiety enhances the binding in aq. soln. compared to a cationically charged deriv. devoid of this functionality. Moreover, with immobilized nucleic acid, binding was obsd. exclusively for the conjugate 1.

IT 22919-50-2, 1-(3-Bromopropyl)thymine
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction with N,N-dimethylaminomethylferrocene)
 RN 22919-50-2 HCAPLUS
 CN 2,4(1H,3H)-Pyrimidinedione, 1-(3-bromopropyl)-5-methyl- (9CI) (CA INDEX NAME)



L48 ANSWER 11 OF 1615 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1996:724551 HCAPLUS
 DOCUMENT NUMBER: 126:47024
 TITLE: Oxidation of 1,3-dimethylthymine with oxone catalyzed by 5,10,15,20-tetrakis(4N-methylpyridiniumyl)porphyrinatomanganese(III) pentaacetate
 AUTHOR(S): Chauhan, S. M. S.; Gupta, Mamta; Gulati, A.; Nizar, P. N. H.
 CORPORATE SOURCE: Dep. Chem., Univ. Delhi, Delhi, 110 007, India
 SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1996), 35B(12), 1267-1270
 CODEN: IJSBDB; ISSN: 0376-4699
 PUBLISHER: Publications & Information Directorate, CSIR
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The title reaction in phosphate buffer gives 1,3-dimethyl-5-hydroxymethyluracil (I), 1,3-dimethyl-5-formyluracil (II), 1,3-dimethyluracil-5-carboxylic acid (III), cis-1,3-dimethylthymine-5,6-glycol (IV), and 1,3,5-trimethyl-5-hydroxybarbituric acid (V) in different yields depending on the pH of the reaction medium. Oxidn. of the 5-Me group of 1,3-dimethylthymine to I, II, and III may be explained by a hydrogen abstraction and recombination mechanism, whereas oxidn. of 5,6-double bond to IV and V may be explained either by electron transfer followed by oxygen atom transfer or by the involvement of hydroxy radicals.
 IT 14181-46-5P, 1,3-Dimethyl-5-hydroxymethyluracil
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (oxidn. of dimethylthymine with pyridiniumylporpyrinatomanganese catalyst)
 RN 14181-46-5 HCAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 5-(hydroxymethyl)-1,3-dimethyl- (9CI) (CA INDEX NAME)



L48 ANSWER 12 OF 1615 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1996:685314 HCAPLUS
 DOCUMENT NUMBER: 125:329288
 TITLE: Preparation of ansacytidine and ansacytosine derivatives as drugs.
 INVENTOR(S): Vorbrueggen, Helmut; Krolikiewicz, Konrad; Schirner, Michael; Schneider, Martin; Wiesinger, Herbert
 PATENT ASSIGNEE(S): Schering A.-G., Germany
 SOURCE: Ger. Offen., 14 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19514523	A1	19961017	DE 1995-19514523	19950412
WO 9632403	A2	19961017	WO 1996-EP1595	19960412
WO 9632403	A3	19961128		

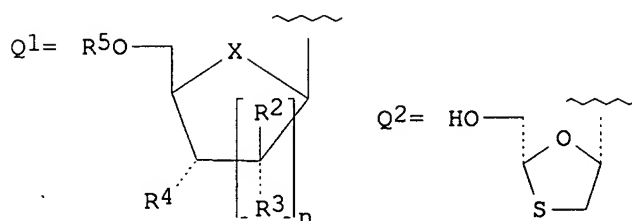
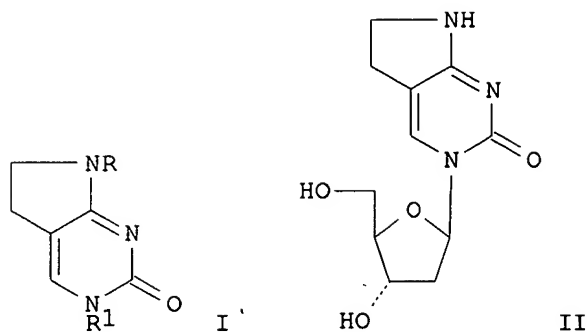
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RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

AU 9654000	A1	19961030	AU 1996-54000	19960412
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PRIORITY APPLN. INFO.: DE 1995-19514523 19950412
 WO 1996-EP1595 19960412

OTHER SOURCE(S): MARPAT 125:329288
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AB Title compds. [I; R = H, CHO, COR₆; R₆ = alkyl, Ph, CO₂R₇; R₇ = alkyl, PhCH₂; R₁ = H, Q₁, Q₂, CH₂CH₂OCH₂CH₂OH, CH₂CH(CH₂OH)₂, CH₂CH₂CH(CH₂OH)OCH₂PO(OH)₂; n = 1, 2; X = O, S, CH₂, imino; R₂ = H, F, Me, CN; R₃ = H, F, OH, OMe; R₄ = H, F, OH, N₃, NH₂; R₅ = H, PO(OH)₂; R₂R₃ = CH₂; R₃R₄ = bond], were prepd. as anticancer and antiviral agents (no data). Thus, 7-acetyl-3,5,6,7-tetrahydro-2h-pyrrolo[2,3-d]pyrimidin-2-one (prepn. given) was refluxed with Me₃SiCl and (Me₃Si)₂NH in MeCN to give the corresponding silyl enol ether deriv., which in ClCH₂CH₂Cl was treated with 3,5-Di-O-toluoyl-2-desoxy-.alpha.-D-ribofuranosyl chloride and trimethylsilyl triflate to give a mixt. of .alpha.- and .beta.-coupling products. The .beta.-anomer was deprotected with NH₃ in MeOH to give title compd. (II). II is said to be esp. suitable for formation of stable triplex DNA.

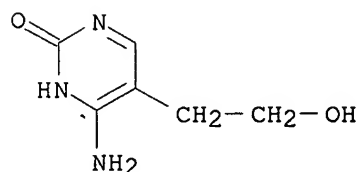
IT **89711-99-9**

RL: RCT (Reactant)

(prepn. of ansacytidine and ansacytosine derivs. as drugs)

RN 89711-99-9 HCAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-5-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)



L48 ANSWER 13 OF 1615 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:657130 HCAPLUS

DOCUMENT NUMBER: 126:8490

TITLE: Photosensitized Oxidation of 5-Methyl-2'-deoxycytidine

by 2-Methyl-1,4-naphthoquinone: Characterization of 5-(Hydroperoxymethyl)-2'-deoxycytidine and Stable Methyl Group Oxidation Products

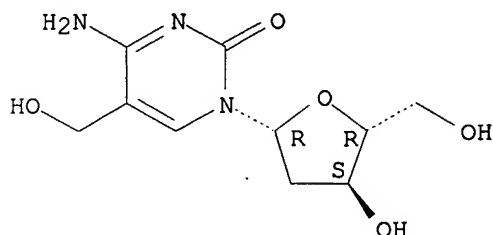
AUTHOR(S): Bienvenu, Carine; Wagner, J. Richard; Cadet, Jean
 CORPORATE SOURCE: Departement de Recherche Fondamentale sur la Matiere Condensee, CEA-Grenoble, Grenoble, F-38054, Fr.
 SOURCE: Journal of the American Chemical Society (1996), 118(46), 11406-11411
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 126:8490

AB UV-A irradiation of an aerated aq. soln. of 5-methyl-2'-deoxycytidine in the presence of menadione (MQ) as a type I photosensitizer leads to the formation of several stable oxidn. products. Emphasis was placed in this study on the isolation and the characterization of the major class of decompn. products whose formation involves the oxidn. of the Me group. These include 5-(hydroperoxymethyl)-2'-deoxycytidine and two stable decompn. products namely, 5-(hydroxymethyl)-2'-deoxycytidine and 5-formyl-2'-deoxycytidine. Structural assignment of the latter modified nucleosides was inferred from extensive spectroscopic measurements (1H and 13C NMR, UV spectroscopy, and mass spectrometry). In addn., conformational anal. of the oxidized nucleosides was inferred from detailed 1H NMR anal. All of the above photooxidn. products appear to arise from the deprotonation of the 5-methyl-2'-deoxycytidine radical cation which is generated by menadione photosensitization.

IT 7226-77-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (photosensitized oxidn. of methyldeoxycytidine by methyl-naphthoquinone and characterization of hydroperoxymethyldeoxycytidine and stable Me group oxidn. products)

RN 7226-77-9 HCAPLUS
 CN Cytidine, 2'-deoxy-5-(hydroxymethyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



L48 ANSWER 14 OF 1615 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1996:616114 HCAPLUS
 DOCUMENT NUMBER: 125:275154
 TITLE: Derivatives of Dihydropyrazine-1,4-Dioxide, 3-Imidazoline 3-Oxide, and .alpha.-Phenyl Nitrones with Functional Groups as New Spin Traps in Solution and in the Gas Phase

AUTHOR(S): Dultseva, Galina G.; Skubnevskaya, Galina I.;
Tikhonov, Aleksei Ya.; Mazhukin, Dmitrii G.;
Volodarsky, Leonid B.

CORPORATE SOURCE: Institute of Chemical Kinetics and Combustion,
Novosibirsk, 630090, Russia

SOURCE: J. Phys. Chem. (1996), 100(44), 17523-17527
CODEN: JPCHAX; ISSN: 0022-3654

DOCUMENT TYPE: Journal

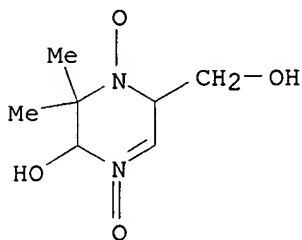
LANGUAGE: English

AB The title compds., acyclic Ph nitrones with functional groups, cyclic
dinitrones with conjugated or isolated double bonds, and imidazoline
nitrones are studied as spin traps (ST) for short-lived free radicals (R)
generated photochem. in soln. and in the gas phase. New STs are efficient
in trapping OH, hydroxyalkyl, or HO2 radicals. EPR spectra of the spin
adducts (SA) of studied dinitrones are triplets of doublets characteristic
of the nitroxides with one radical center. Imidazoline ST with amino
nitrogen exhibits pH-dependent hyperfine splittings of its SAs. Some spin
traps were shown to be efficient in detecting R in the atm. expts.

IT 123194-14-9 123194-16-1 123194-18-3
182323-02-0 182323-05-3
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation,
nonpreparative)
(spin traps for short-lived free radicals generated photochem. in soln.
and in the gas phase)

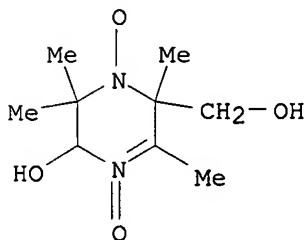
RN 123194-14-9 HCAPLUS

CN 1(2H)-Pyrazinyloxy, 3,6-dihydro-3-hydroxy-6-(hydroxymethyl)-2,2-dimethyl-,
4-oxide (9CI) (CA INDEX NAME)



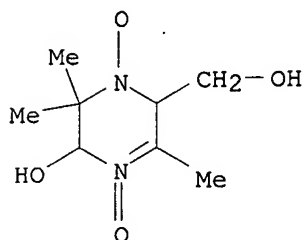
RN 123194-16-1 HCAPLUS

CN 1(2H)-Pyrazinyloxy, 3,6-dihydro-3-hydroxy-6-(hydroxymethyl)-2,2,5,6-
tetramethyl-, 4-oxide (9CI) (CA INDEX NAME)



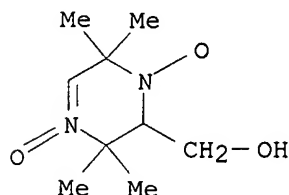
RN 123194-18-3 HCAPLUS

CN 1(2H)-Pyrazinyloxy, 3,6-dihydro-3-hydroxy-6-(hydroxymethyl)-2,2,5-trimethyl-, 4-oxide (9CI) (CA INDEX NAME)



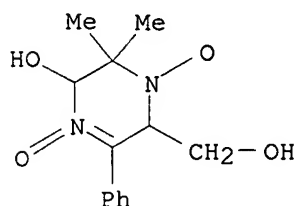
RN 182323-02-0 HCAPLUS

CN 1(2H)-Pyrazinyloxy, 5,6-dihydro-6-(hydroxymethyl)-2,2,5,5-tetramethyl-, 4-oxide (9CI) (CA INDEX NAME)



RN 182323-05-3 HCAPLUS

CN 1(2H)-Pyrazinyloxy, 3,6-dihydro-3-hydroxy-6-(hydroxymethyl)-2,2-dimethyl-5-phenyl-, 4-oxide (9CI) (CA INDEX NAME)



L48 ANSWER 15 OF 1615 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:613912 HCAPLUS

DOCUMENT NUMBER: 125:301481

TITLE: Synthesis of some aminonaphthalene and 5-substituted uracil nucleosides derivatives

AUTHOR(S): Ahmed, A. F. Sayed; Milad, A.

CORPORATE SOURCE: Faculty Science, Zagazig University, Zagazig, Egypt

SOURCE: Chim. Acta Turc. (1996), 24(2), 101-104

CODEN: CATUA9; ISSN: 0379-5896

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Some amino naphthalene nucleosides were prepd. by the reaction of both of 1-amino, 1-aminomethyl, 1,5-diamino and 2,6-bis (aminomethyl) naphthalene

derivs. with 2, 3, 5-tri-O-acetyl ribofuranosyl chloride. On the other hand, the reactions of 2',3'-O-isopropylidene-5-aminouridine and its 5-aminomethyl analog with gluconolactone and the reactions of 2',3'-O-isopropylidene-5-chloromethyl uridine with sodium N-Me taurinate have been described.

IT 89148-09-4

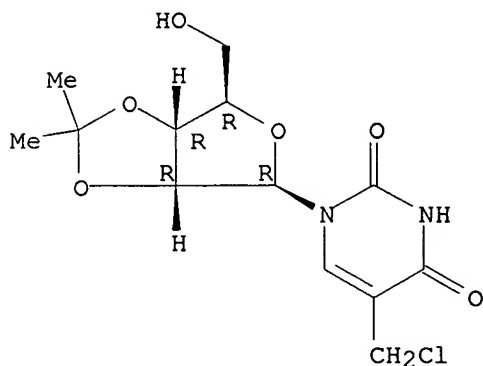
RL: RCT (Reactant)

(prepn. of amino naphthalene nucleosides)

RN 89148-09-4 HCAPLUS

CN Uridine, 5-(chloromethyl)-2',3'-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L48 ANSWER 16 OF 1615 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:611068 HCAPLUS

DOCUMENT NUMBER: 125:294828

TITLE: Urinary excretion of 5-hydroxymethyluracil as indicator of oxidative DNA damage and repair

AUTHOR(S): Bianchini, F.; Cadet, J.

CORPORATE SOURCE: Departement de la Recherche Fondamentale sur la Matiere Condensee, CEA/Grenoble, Grenoble, 38054/9, Fr.

SOURCE: Spec. Publ. - R. Soc. Chem. (1996), 181 (Natural Antioxidants and Food Quality in Atherosclerosis and Cancer Prevention), 73-77
CODEN: SROCD0; ISSN: 0260-6291

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A method was developed for the detn. of 5-hydroxymethyluracil (5-HMUra) and the corresponding nucleoside 5-HMdUrd, and application to human samples is presented. The method is based on HPLC prepurifn. of urine and gas chromatog./mass spectrometry anal. of the modified nucleobase or nucleoside. Only 1 mL urine is needed for anal., and the exptl. variability is extremely low. Also, the level of urinary 5-HMUra seems to be different between individuals, while it is sufficiently stable with time for the same individual.

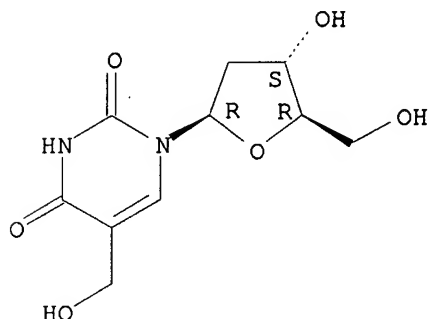
IT 5116-24-5, 5-Hydroxymethyl-2'-deoxyuridine

RL: ANT (Analyte); ANST (Analytical study)

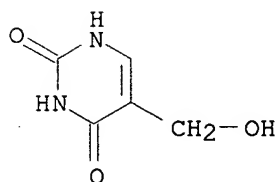
(urinary excretion of 5-hydroxymethyluracil as indicator of oxidative DNA damage and repair)

RN 5116-24-5 HCAPLUS
 CN Thymidine, .alpha.-hydroxy- (9CI) (CA INDEX NAME)

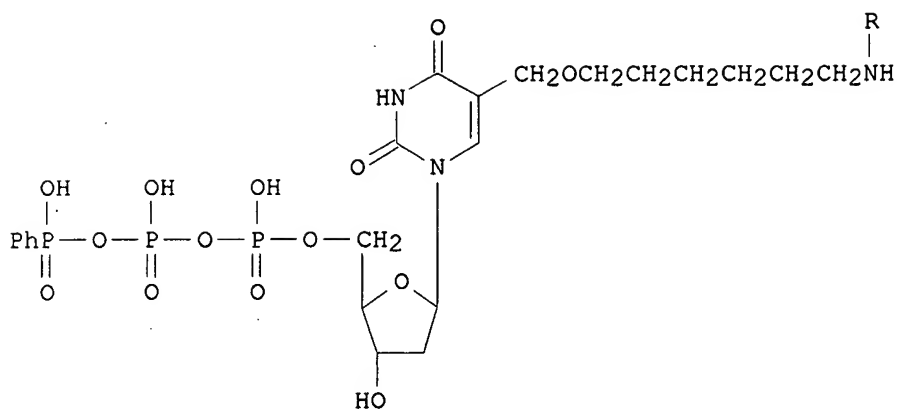
Absolute stereochemistry.



IT 4433-40-3, 5-Hydroxymethyluracil
 RL: ANT (Analyte); BPR (Biological process); ANST (Analytical study); BIOL (Biological study); PROC (Process)
 (urinary excretion of 5-hydroxymethyluracil as indicator of oxidative DNA damage and repair)
 RN 4433-40-3 HCAPLUS
 CN 2,4(1H,3H)-Pyrimidinedione, 5-(hydroxymethyl)- (9CI) (CA INDEX NAME)



L48 ANSWER 17 OF 1615 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1996:600923 HCAPLUS
 DOCUMENT NUMBER: 125:329243
 TITLE: Nucleoside 5'-triphosphates modified at both nucleic base and triphosphate moiety
 AUTHOR(S): Alexandrova, L. A.; Scoblov, A. Yu.
 CORPORATE SOURCE: Engelhardt Institute Molecular Biology, Russian Academy Sciences, Moscow, 117984, Russia
 SOURCE: Collect. Czech. Chem. Commun. (1996), 61(Spec. Issue), S156-S157
 CODEN: CCCCAK; ISSN: 0010-0765
 DOCUMENT TYPE: Journal
 LANGUAGE: English
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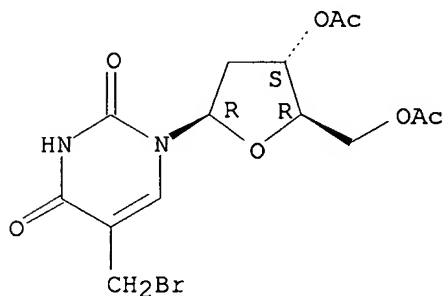
AB Nucleoside 5'-triphosphates modified at the triphosphate moiety and contg. reporter groups at the C5 position of 2'-deoxyuridine were synthesized. The target compds. were the UTP derivs. I (R = reporter group). The structure of these compds. was confirmed by NMR and mass spectroscopy.

IT **58589-18-7**, 5-(Bromomethyl)-2'-deoxy-3',5'-di-O-acetyluridine
 RL: RCT (Reactant)
 (prepn. of 5,5'-modified uridine triphosphates)

RN 58589-18-7 HCAPLUS

CN Thymidine, .alpha.-bromo-, 3',5'-diacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L48 ANSWER 18 OF 1615 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:600893 HCAPLUS

DOCUMENT NUMBER: 125:300682

TITLE: New application of the Stille coupling in the synthesis of 5-substituted uracils

AUTHOR(S): Wagner, Roman; Dvorak, Dalimil; Holy, Antonin

CORPORATE SOURCE: Institute Organic Chemistry Biochemistry, Academy Sciences Czech Republic, Prague, 166 10, Czech Rep.

SOURCE: Collect. Czech. Chem. Commun. (1996), 61(Spec. Issue), S118-S119

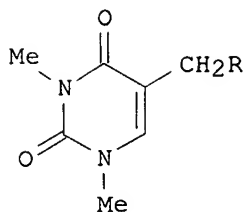
CODEN: CCCCCA; ISSN: 0010-0765

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 125:300682

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AB Stille coupling of 5-chloromethyl-1,3-dimethyluracil and the appropriate tributyltin deriv. in the presence of Pd2dba3 and Ph3As gave the title compds. I (R = vinyl, ethynyl, Ph) in satisfactory yields.

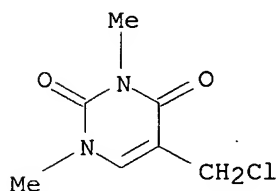
IT 32079-06-4

RL: RCT (Reactant)

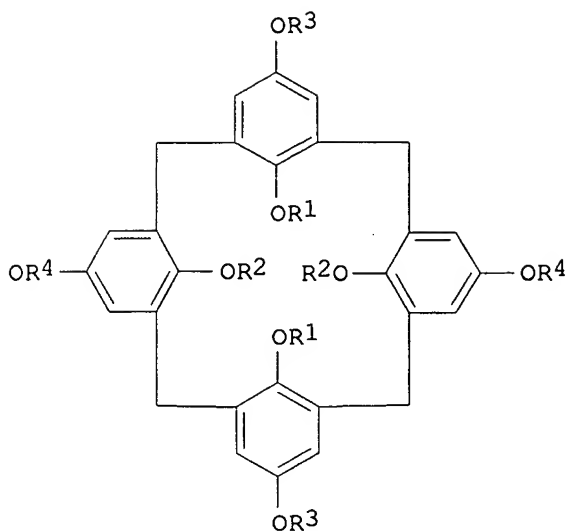
(prepn. of 5-substituted uracils via the Stille coupling)

RN 32079-06-4 HCAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 5-(chloromethyl)-1,3-dimethyl- (9CI) (CA INDEX NAME)



L48 ANSWER 19 OF 1615 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1996:592044 HCAPLUS
 DOCUMENT NUMBER: 125:275817
 TITLE: Aggregates of calix[4]arenes based on the
 2,6-diaminotriazine.cntdot.imide system
 AUTHOR(S): Vreekamp, Remko H.; Verboom, Willem; Reinhoudt, David
 N.
 CORPORATE SOURCE: Laboratory of Organic Chemistry, University of Twente,
 Enschede, Neth.
 SOURCE: Recl. Trav. Chim. Pays-Bas (1996), 115(7/8), 363-370
 CODEN: RTCPA3; ISSN: 0165-0513
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



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AB The synthesis of several calix[4]arenes functionalized with uracil or diaminotriazine moieties is described. The assocn. between these complimentary calix[4]arenes is strongly influenced by processes related to the position and directionality of the hydrogen-bound moieties. In the case of bis(uracil)calix[4]arene I [R1 = H, R2 = (2,4(1H,3H)-dioxypyrimidine-6-yl)methyl, R3 = R4 = hexyl], self-assocn. is obsd. (K = 3.4 .times. 10³ M⁻¹ in CDCl₃). In the case of bis(diamidotriazine)calix[4]arene I [R1 = R2 = Pr, R3 = 4-(hexanoylamino)-6-amino-1,3,5-triazin-2-yl, R4 = H], it was concluded from 1H-NMR studies that intermol. assocn. is hampered by the formation of intramol. hydrogen bonds. Due to the divergent orientation of the hydrogen-bonding groups of bis(diaminotriazine)calix[4]arene I (R1 = R2 = Pr R3 = 4,6-diamino-1,3,5-triazin-2-yl, R4 = H), it forms hydrogen-bonded strands through interaction with 5-ethyl-5-phenylbarbituric acid, resulting in the formation of a gel in chloroform.

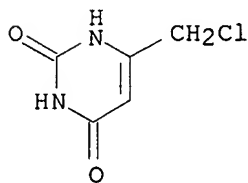
IT **18592-13-7**, 6-(Chloromethyl)uracil

RL: RCT (Reactant)

(aggregates of calix[4]arenes based on the diaminotriazine-imide system)

RN 18592-13-7 HCAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 6-(chloromethyl)- (9CI) (CA INDEX NAME)



dis. Clamant

DOCUMENT NUMBER: 125:214607
TITLE: Base modification and strand breakage in isolated calf thymus DNA and in DNA from human skin epidermal keratinocytes exposed to peroxyxynitrite or 3-morpholinolinosydnnonimine
AUTHOR(S): Spencer, Jeremy P. E.; Wong, Jon; Jenner, Andrew; Aruoma, Okezie I.; Cross, Carroll E.; Halliwell, Barry
CORPORATE SOURCE: Neurodegenerative Disease Research Centre, University of London King's College, London, SW3 6LX, UK
SOURCE: Chemical Research in Toxicology (1996), 9(7), 1152-1158
CODEN: CRTOEC; ISSN: 0893-228X
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Exposure of isolated calf thymus DNA and human skin epidermal keratinocytes to peroxyxynitrite or the peroxyxynitrite generator, 3-morpholinolinosydnnonimine (SKIN-1), led to extensive DNA base modification. Large increases in xanthine and hypoxanthine, possible deamination products of guanine and adenine, resp., and in 8-nitroguanine were obsd., but only small changes in some oxidized base products were seen. This pattern of damage suggests that hydroxyl radicals were not major contributors to base modification caused by peroxyxynitrite, as OH.bul. is known to cause multiple oxidative modifications to all four DNA bases. Instead, it seems that reactive nitrogen species play a much greater role in the mechanism of base damage, producing both nitration and deamination of purine bases when DNA or whole cells are exposed to peroxyxynitrite. If this pattern of damage is unique to peroxyxynitrite, it might act as a marker of cellular damage by this species in vivo.
IT 4433-40-3, 5-Hydroxymethyluracil
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(base modification and strand breakage in thymus DNA and in DNA from human skin epidermal keratinocytes exposed to peroxyxynitrite or 3-morpholinolinosydnnonimine)
RN 4433-40-3 HCAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 5-(hydroxymethyl)- (9CI) (CA INDEX NAME)

